On the isotropic Raman spectrum of Ar2 and how to benchmark ab initio calculations of small atomic clusters: Paradox lost

Titre	On the isotropic Raman spectrum of Ar2 and how to benchmark ab initio calculations of small atomic clusters: Paradox lost
Type de publication	Article de revue
Auteur	Chrysos, Michel [1], Dixneuf, Sophie [2], Rachet, Florent [3]
Pays	Etats-Unis
Editeur	American Institute of Physics
Ville	Melville
Type	Article scientifique dans une revue à comité de lecture
Année	2015
Langue	Anglais
Date	14/07/2015
Numéro	2
Pagination	024304
Volume	143
Titre de la revue	The Journal of Chemical Physics
ISSN	0021-9606
Mots-clés	Ab initio calculations [4], Atomic spectra [5], basis sets [6], Polarizability [7], Raman spectra [8]
Résumé en français	This is the long-overdue answer to the discrepancies observed between theory and experiment in Ar_2 regarding both the isotropic Raman spectrum and the second refractivity virial coefficient, B_R [Gaye et al., Phys. Rev. A 55, 3484 (1997)]. At the origin of this progress is the advent (posterior to 1997) of advanced computational methods for weakly interconnected neutral species at close separations. Here, we report agreement between the previously taken Raman measurements and quantum lineshapes now computed with the employ of large-scale CCSD or smartly constructed MP2 induced-polarizability data. By using these measurements as a benchmark tool, we assess the degree of performance of various other ab initio computed data for the mean polarizability α, and we show that an excellent agreement with the most recently measured value of B_R is reached. We propose an even more refined model for α, which is solution of the inverse-scattering problem and whose lineshape matches exactly the measured spectrum over the entire frequency-shift range probed.
URL de la notice	http://okina.univ-angers.fr/publications/ua13520 [9]
DOI	10.1063/1.4923370 [10]
Lien vers le document	http://dx.doi.org/10.1063/1.4923370 [10]

Titre abrégé	J. Chem. Phys.

Liens
[1] http://okina.univ-angers.fr/michel.chrysos/publications
[2] http://okina.univ-angers.fr/publications?f[author]=16738
[3] http://okina.univ-angers.fr/florent.rachet/publications
[4] http://okina.univ-angers.fr/publications?f[keyword]=4932
[5] http://okina.univ-angers.fr/publications?f[keyword]=4934
[6] http://okina.univ-angers.fr/publications?f[keyword]=19683
[7] http://okina.univ-angers.fr/publications?f[keyword]=4937
[8] http://okina.univ-angers.fr/publications?f[keyword]=19682
[9] http://okina.univ-angers.fr/publications/ua13520
[10] http://dx.doi.org/10.1063/1.4923370